DOE CHEMICAL ANALYSIS MARKET AND PRACTICES: FOCUSING ON NEEDS FOR ANALYSIS AUTOMATION IN ENVIRONMENTAL MANAGEMENT OPERATIONS

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ABSTRACT

This report documents chemical analysis practices and needs at five major U.S. Department of Energy (DOE) Operations Offices (Savannah River, Richland, Oak Ridge, Rocky Flats, and Idaho) and the Fernald site, which is under the jurisdiction of the DOE Ohio Operations Office. The combined, operational budgets of these sites account for about 70 percent of the FY 1998 adjusted budget of the Office of Environmental Management (EM), which is responsible for managing waste and cleaning up contamination at DOE sites across the nation. In addition, these sites cover the spectrum of DOE-EM operations, comprising two sites (Fernald and Rocky Flats) on the accelerated path to closure by the year 2006 and four sites (those remaining) with operations continuing after 2006. Thus, the practices and needs of these sites can well represent the overall analytical service operations in support of the DOE-EM cleanup mission, both in the near term and in the long term.

The survey findings indicated that by first approximation the DOE-EM complex-wide analytical service market is estimated at $114 million per year, with a yearly sample load of 284,000 samples. Although both the overall market and sample load offer significant potential for analysis automation, many different analysis methods are being employed at DOE sites because of varying sample characteristics and analysis/reporting requirements. Potential for analysis automation exists only in niche areas; notably, these include radiochemical analysis, metal analysis, and sample preparation.

INTRODUCTION

The complexity of individual DOE site wastes and the accompanying variety of related analytical methods and procedures makes it an aimless task to cover each analytical practice. Instead, this report is intended to capture the "big-picture" information about DOE-EM analytical services, especially that of relevance to potential applications of analysis automation. It is recognized that the inherent need for automation must be justified by a significant quantity of practices and by a significant improvement of performance in consistency of data quality and in timely turnaround service; therefore, this report approaches the analysis automation demand from both the "quantity" and "quality" perspectives.

The quantity and quality aspects of the information, obtained through surveys conducted individually at these sites and used to assess the analysis automation demand, are grouped into the following categories:

- analytical budget,
- samples projection,
- fast turnaround analysis demand,
- the ten costliest analytical services (product of unit cost and number of samples), and
- quality of current practices and site-perceived needs for analysis automation.

This paper will present the site survey results by each of the above categories.

SITE SURVEY RESULTS AND DISCUSSIONS

Information for this report was gathered by first searching and collecting historical site analytical service information, then conducting site visits to interview responsible site personnel for up-to-date information and their views of future analysis demand, followed by additional data collection via follow-up telephone surveys. The individual survey results were then sent to their corresponding sites to obtain feedback, which was incorporated in the results presented below. These results are grouped by each category mentioned above, with a brief summary of individual site results and assessment of the extrapolated DOE-EM complex-wide demand. More detailed information about each surveyed site can be found in a recently published report.(1)

To obtain an estimate for the DOE-EM complex-wide demand, the cumulative results of both the analytical budget amounts and sample number projections of these six surveyed sites were each divided by a 70-percent factor, which is approximately the ratio of the cumulative overall budget of the six sites to the overall DOE-EM budget. By first approximation, this 70-percent factor is assumed to be equivalent to the ratio of the cumulative analytical services at these sites to the DOE-EM complex-wide analytical services.

Analytical Budget

Complete budget information for analytical services was obtained from four sites, with only partial budget information obtained from the remaining two. The site budgets are listed in Table I, which shows that the overall annual budget for analytical services at the surveyed sites is estimated to be close to $80 million, after including estimated amounts for the missing portion of the Savannah River and Idaho budget information. Assuming a 1:1 correspondence between the DOE-EM budget and the DOE-EM analytical service budget (i.e., the surveyed sites also account for 70 percent of the DOE-EM analytical service budget), the DOE-EM complex-wide analytical service budget can be extrapolated to $114 million a year, using the known, individual site budget averages of 1998 and 1999.

Table I. Annual Analytical Service Budget at Six DOE Sites, Based on an Average of FY 1997 and 1998 Results

DOE Survey Site	**Analytical Service Budget ($M/Year)**
Richland	39
Idaho	10 (only on-site laboratory operations)
Savannah River	7.6 (only the environmental restoration portion of analytical services)
Rocky Flats	7
Oak Ridge	6.1
Fernald	3.8
Idaho/Savannah River (estimated for the remainder of site analytical services)	6.3
Total of the Six Sites	80
Total, DOE-EM	114*

* $114 M = $80 M / 0.7, assuming that the surveyed sites account for 70 percent of the DOE-EM analytical service budget

The estimated $114 million in DOE-EM annual analytical service operations is lower than the estimate of more than $200 million per year reported elsewhere.(2) An attempt to obtain background information from the Integrated Performance Evaluation Program for the $200 million estimate was unsuccessful because the information database was being restructured, and no breakout of the $200 million by site was available. Although the cause of the discrepancy between these two estimates is not known, one assumption is that the higher estimate would have been obtained from data prior to FY 1997. This is supported by the finding that all of the surveyed sites expressed that their analytical budgets started to stabilize around FY 1997 from an earlier declining curve. The two sites most affected are Richland and Oak Ridge. At Richland, the data quality objective (DQO) approach was widely adopted resulting in a significant reduction in sample analyses; whereas at Oak Ridge, implementation of performance-based procurement in place of fixed-price procurement resulted in a 45-percent improvement in cost effectiveness. Many sites have streamlined their analytical services considerably since the issuance of a 1995 GAO report (3) revealing high analytical costs from the DOE Operations Offices. Such improved practices have been documented in a report stating that "EM's average price for Contract Laboratory Program methods dropped 31% since 1995."(4)

Although the estimated $114 million in DOE-EM annual analytical service operations is deemed a significant market, worth consideration for analysis automation, a significant challenge exists in achieving "significant" cost improvement over the improved current practices. Additionally, introduction of new technologies must overcome the residual effect of the build-up of analytical services that peaked around 1994 and 1995 and resulted in an over capacity in some segments of analytical operations. Therefore, investment in new, automated technologies must be made in the specific application areas where demand outpaces the current capacity.

Samples Projection

Complete sample projections were obtained from all sites except Rocky Flats, which provided the sample projection only for commercial laboratories and not for its on-site hot laboratory. Applying the same extrapolation method used above, the DOE-EM complex-wide demand is about 284,000 samples per year. Water and soil samples are the dominating media, with other media including sludge, debris, etc. The ratio of water to soil samples at these sites averages 1.5:1. Figure 1 depicts the total sample projection by each surveyed site; details about the breakout of each site sample projection by site operation (e.g., environmental restoration, waste management, special projects, etc.) are provided in a separate report.(1)

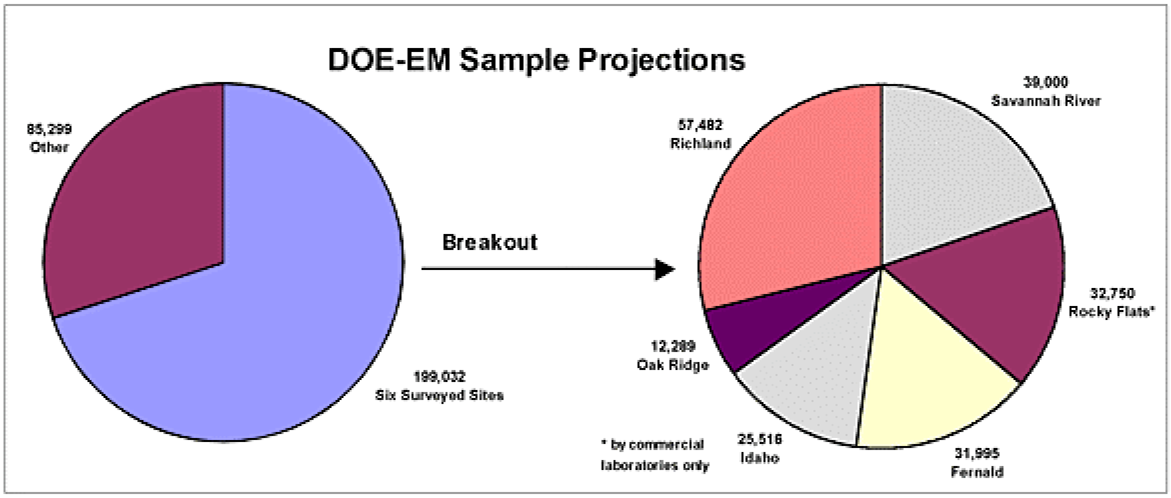

Figure 1. Yearly Analytical Sample Load at DOE Sites, Based on an Average of FY 1997 and FY 1998 Sample Counts

The annual sample load at each DOE site surveyed was also stabilizing around 1997 and 1998 from a declining trend, corresponding with the site analytical service budget. One notable example is the Hanford Site—its sample analysis demand (5), from 1995 through 2003, is shown in Figure 2. The significant reduction of sample demand from the 1995 level, as shown in Figure 2, was attributed to the combination of implemented DQO process, reduced Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) work, and reduced processing support at the Hanford Site. All sites surveyed reported that they expect the sample load to level off or slightly increase from the reported average, shown in Figure 1.

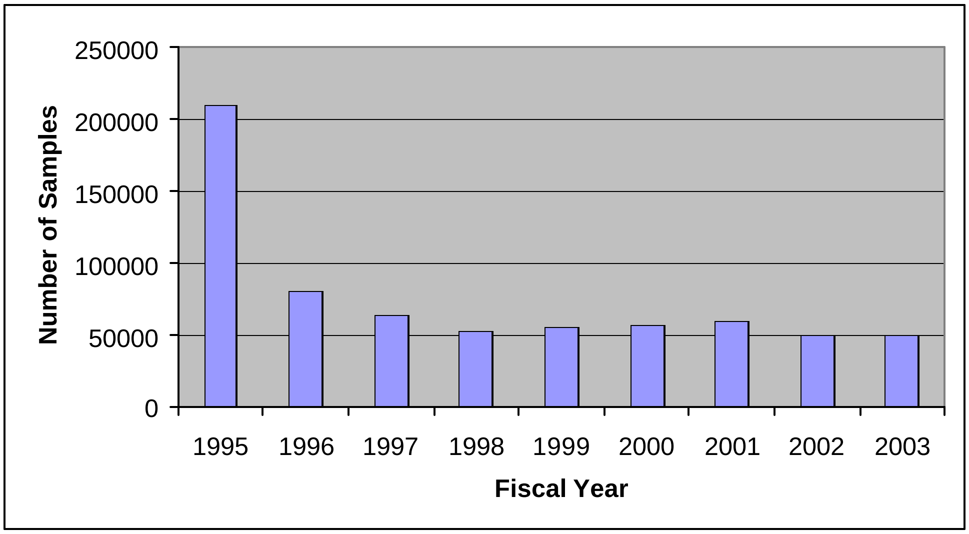

Figure 2. Hanford Sample Analysis Demand, FY 1995 – FY 2003

Many methods are being used at any individual site because of, to name a few important causes, varying radioactivity level, sample matrices, quality control requirements, and sample media (water, soil, sludge, debris, etc.). Although the sample projection numbers in Figure 1 are deemed high, they may not be as good an indicator for the demand of analysis automation as the number of samples associated with each method (or the quantity threshold). Using
3,600 samples per year (i.e., 15 samples per day and 240 days/year) as an arbitrary threshold, the following analyses have been identified to exceed this threshold:

- 16,000 samples for kinetic phosphorescence analysis (KPA) at Fernald,
- 7,647 samples for beryllium analysis at Rocky Flats,
- 7,225 samples for bioassay at Rocky Flats,
- 4,759 and 4,471 samples for gross alpha/beta measurements at Rocky Flats and Hanford, respectively, and
- 3,669 samples for gamma spectroscopy at the Idaho Analytical Laboratory Department Services.

The above list does not include combinations of several current methods into one automated analysis. One such example is Fernald's intent to adopt the inductively coupled plasma mass spectrometry (ICP-MS) technique to replace the atomic emission spectroscopy (AES)/absorption analysis (AA) methods having a combined annual sample load of 4,841. Conceivably, other reasonable combinations may include radiochemical and analytical techniques for radionuclide speciation.

This list also does not capture common practices that crosscut various analyses. Examples in this area include sample preparation techniques that generally are not tracked by sites as a separate entry.

Fast Turnaround Analysis Demand

All except two sites surveyed have arranged to have an adequate capacity for fast turnaround service. Excluding the one-day turnaround analysis of 16,000 water samples per year at Fernald, the number of samples requiring fast turnaround analysis ranges from 15 to 20 percent of the total sample requests. The turnaround practices vary between commercial laboratories and on-site, contractor-operated laboratories.

For all of the contractor-operated laboratories except the Hanford Waste Sampling and Characterization Facility (WSCF), there is no separate charge practice for fast turnaround analyses. Most of these on-site laboratories were designed to handle fast turnaround analyses, difficult matrices, and high radioactivity. The Oak Ridge Sample Management Office directs all sample requests with 24-hour turnaround to its on-site laboratories. Because of their intended purpose, on-site laboratories generally deliver their analytical service results faster than commercial laboratories. For example, the Fernald on-site laboratory completed more than 90 percent of its analyses within 31 days in FY 1998; the standard turnaround at the Hanford WSCF is seven days—the WSCF is the only on-site laboratory that charges a premium of 100 percent for one-day analysis turnaround.

For commercial laboratories, the standard turnaround is 30 days for Savannah River, Oak Ridge, Idaho, and Rocky Flats. For Hanford, it is 15 to 30 days. The premiums for fast turnaround services vary from site to site, with a range of multipliers from 1.1 to 1.25 for 21-day service, 1.3 to 1.5 for 14-day service, 1.28 to 1.8 for seven-day service, 2 for three-day service, and 1.81 to 3 for one-day service. These cost multipliers for fast turnaround services at individual sites are shown in Figure 3.

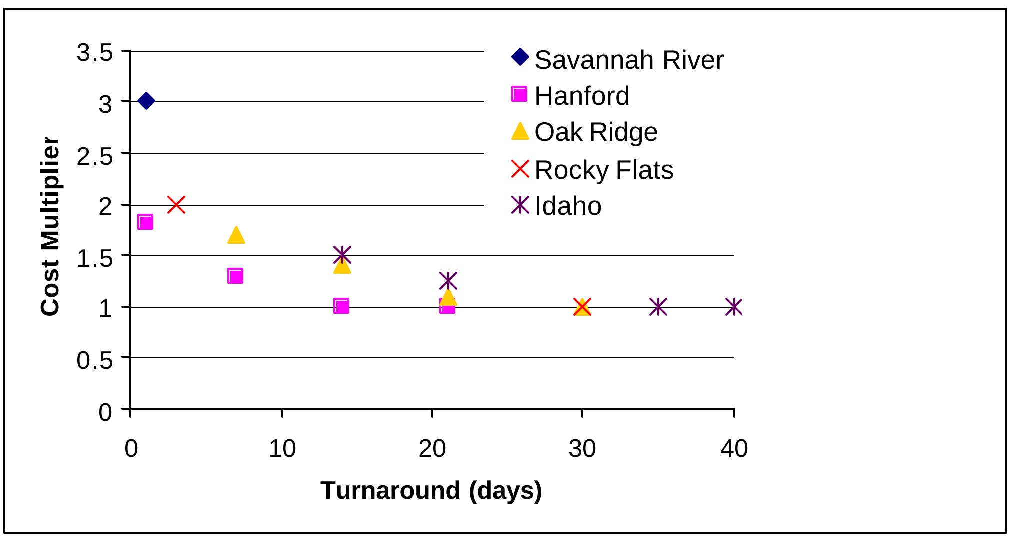

Figure 3. Cost Multiplier for Fast Turnaround Services

In general, all sites except Savannah River have arranged to have an adequate capacity for fast turnaround service. Savannah River is currently expanding the on-site commercial mobile laboratory to increase its capacity for the suite of target analyte list (TAL) and target compound list (TCL) analyses. Although the Fernald Advanced Waste Water Treatment (AWWT) facility laboratory has a capacity for 16,000 water sample analyses per year by KPA, the operation is labor intensive and three shifts are necessary to meet the demand.

The Ten Costliest Analytical Services

A significant variation from site to site exists in how each site compiles and organizes individual sample requests as well as how they implement their charging practices for each request. Cost variables include radioactivity, special handling, number of quality control samples, reporting requirements, fast turnaround service, and waste matrices. Charging practices take into account some or all of the following factors: labor charge, overhead, materials and supplies, other direct charges, sample preparations, and waste disposal. There is not a common practice among sites for computing costs for each analysis; furthermore, a direct comparison of costs of individual analyses from different sites is not the intent of this study.

The ten costliest analyses (product of unit cost and number of samples) at individual sites are listed in a separate report (except that for Savannah River, whose data was not obtained).(1) Instead of displaying a disparate array of information, a more meaningful way has been employed that groups individual methods into the major compound or parameter classes, allowing the relative significance of each compound or parameter class to be more accurately portrayed. Purposely excluded from this grouping are the special operations performed by the on-site hot laboratories (specifically, the 222-S laboratory at Richland, the Analytical Laboratory Department Services at Idaho, and the hot laboratory for Waste Isolation Pilot Plant, or WIPP, analysis at Rocky Flats). These hot laboratories mostly involve hot-cell operations, which by themselves fall into special areas of analysis automation.

Thus, the relative significance of each individual compound or parameter class is shown in Figure 4 and is also listed below, with the percent of aggregate total annual costs computed from the identified ten costliest analyses in parenthesis:

- Radioactivity and Radiochemical Analysis (45%)
  - Radiochemistry, Gross Alpha/Beta, Gamma Spectroscopy, Isotopic Analyses (U, Pu, Am, Th), Strotium-90, Technetium-99
- Metals (30%)
  - Metals, CLP Metals, TCLP Metals, AA Metals, ICP Metals, Trace Metals by ICP-MS (6020), Total U—ICP/MS, Total U in Water—KPA and Syntrex, Beryllium Swipes
- Semivolatile Organic Compounds (10%)
  - Semivolatile Organic Compounds, SVOCs by gas chromatography/mass spectrometry (GC/MS) (8270B), TCLP Semivolatiles, Pesticides, Herbicides, Polychlorinated Biphenyl (PCB)
- Volatile Organic Compounds (8%)
  - Volatile Organic Compounds, VOCs by GC/MS (8260A), TCLP Volatiles
- Sample Preparation (4%)
  - Preparation, Dry/Grind/% Moisture, TCLP Extractions

- Wet Chemistry/Anions (3%)
  - Wet Chemistry, Anions by Ion Chromatography, Water Quality (Cl, NO2, and NO3)

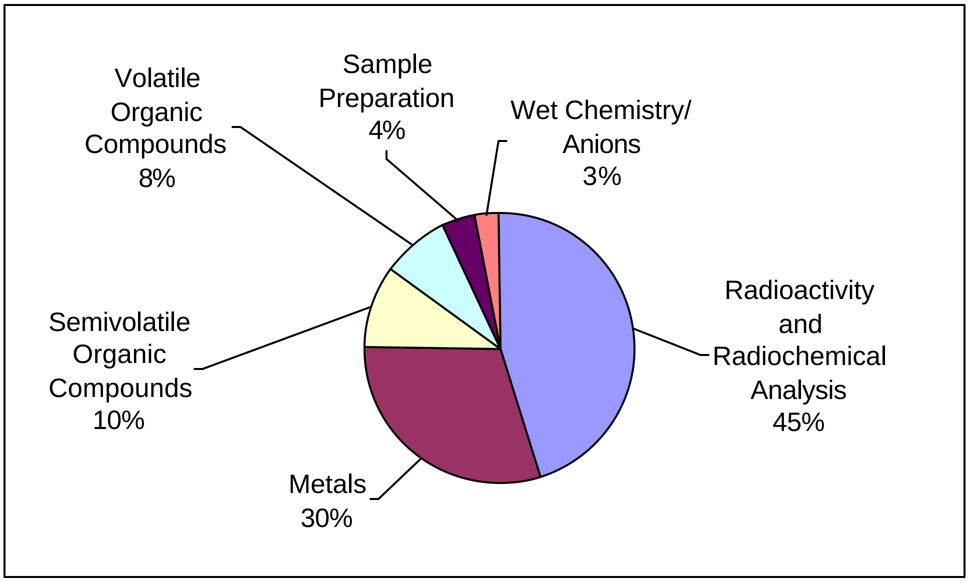

Figure 4. Relative Significance of Each Individual Compound or Parameter Class at DOE Sites, Derived from the Ten Costliest Analytical Services

Of note is the high percentage of site costs associated with radioactivity and radiochemical analysis, even after the hot-cell operations were excluded (i.e., the above percents are calculated based on the low- and no-activity waste analyses only). Again, the groupings above only take into account the ten costliest analyses at individual sites (excluding Savannah River because such data were not obtained), not the entire site analytical service operations. Also of note is that only Fernald and Oak Ridge separate out some of the sample preparation costs; the other sites include sample preparation costs as part of the individual sample analysis costs—thus, the percent of sample preparation costs could conceivable be much higher than indicated.

Quality of Current Practices and Site-Perceived Needs for Analysis Automation

The quality of current practices from on-site and commercial laboratories is a subjective measure, and often if the quality is unsatisfactory, the analytical service manager will seek out alternative suppliers or services. Therefore, the quality of practices and user-perceived need are interrelated.

Fernald has expressed several compelling needs for automation. Many routine, on-site analyses for metals and radiochemical analyses must be carried out to meet the site accelerated closure schedule while the site is facing a declining workforce. These routine operations involve potential hazards to workers from acid fumes and burns during acid digestion of soil samples for uranium, thorium, and other metal analyses. Additionally, a significant portion of Fernald analyses involves remediation verification; therefore, about 30 percent of its analyses require data package documentation, for which Fernald has also expressed a need for automation. Based on both the quantity and quality criteria described above, Fernald's applications are a good candidate for analysis automation. These needs also become pressing as the Fernald on-site laboratory is scheduled to be vacated in FY 2002 in preparation for its planned demolition the following year.

Savannah River has two needs for analysis automation. One need is related to fast turnaround analyses required during precision excavation of the chemical, metals, and pesticides (CMP) pit. Timely and quality analysis is valued by the site remediation project managers to enable minimization of waste generation and work idle time. However, this need is modest, considering the limited quantity of samples requiring analyses. Also, this need could conceivable be addressed by the current capabilities of the Chemical Analysis Automation (CAA) semivolatiles system. The CAA system was previously demonstrated at an Oak Ridge site for automated analysis capabilities for PCBs in soil (6), and this system is being further developed to address analysis needs for a full suite of semivolatile organic compounds.

The other Savannah River need is related to the expansion of its on-site commercial laboratory capacity for fast turnaround TAL/TCL analyses. The on-site commercial laboratory operated by GEL handles only 20 to 25 percent of environmental restoration samples. Based on its significant cost advantage compared to off-site laboratories ($699 versus $2,550 per sample), there is enough cost incentive to increase the percentage of environmental samples that could be handled by the on-site commercial laboratory. Analysis automation could be viable for consideration, and Savannah River is interested in keeping this option open. The potential cost savings were calculated to be $47 million, when the cost differential is applied to all applicable operable units requiring full TAL/TCL characterization.(7) This cost savings potential, however, is not specifically limited to analysis automation developed by the CAA team.

In contrast to Fernald and Savannah River, the other four sites have not expressed current needs for analysis automation. Richland's needs may change depending on decisions about who will be responsible for performing analyses in support of the BNFL glass plant operation—the Phase I proof-of-principle study will begin in FY 2005/2006. Rocky Flats adopted a different approach than Fernald's, and the site has closed out many of its laboratories and has already contracted all non-WIPP-waste analyses to commercial laboratories. Both Oak Ridge and Idaho operations have significantly improved their analytical operations through a privatization effort, and they are content with their current practices.

CONCLUSIONS

As the complex-wide demand is stabilizing and some major improvements in analytical services have already reached fruition, where is the next wave of opportunities for improvement? Most opportunities are in niche areas requiring special attention and penetration to a particular site/user need. The unveiling of the Fernald and Savannah River needs is the epitome of penetrating such niche markets. Both site needs for analysis automation would not have been revealed without a local champion at each site and the dedicated effort of the technology team in exploring such needs.

The sample projection analysis did not show a significantly "high" yearly demand for many singular analyses like KPA at Fernald and beryllium analysis at Rocky Flats. One niche area in system integration as expressed by Fernald is to combine the two current practices of metal analysis techniques

(AA and ICP-AES) into one automated technique (ICP-MS) to provide enough sample demand to warrant new equipment investment. Such practices shall be further explored with other sites in the two highest cost classes, i.e., radioactivity/radiochemical analysis and metals.

Besides this potential system integration niche area, another niche area may exist in modular component automation, specifically in those areas crosscutting many analysis needs. Examples include sample preparation techniques such as grinding, drying, homogenization, weighing, digestion, filtration, dilution, etc., as well as data package documentation. The potential application of automation in sample preparation is wide, in view of all soil and water samples requiring some of these steps before any subsequent analysis. As to data package documentation, it is required for any remedial and waste verification reporting.

Such niche areas don't typically show up in the site cost screen as a separate entry, and close interaction with site users is necessary to uncover the specifics of such needs. A thorough survey of commercial capabilities in modular component automation must be conducted to identify viable niche areas for automation development; and, this development must be done in close collaboration with commercial entities.

In summary, the niche areas for analysis automation in DOE-EM analytical services are identified to include the following:

- In the area of analytical system integration, reasonably combining different analysis techniques currently in use for radioactivity/radiochemical/metal determination into one automated system.
- In the area of modular automation, focusing on elements commonly required for all analyses such as sample preparation procedures including grinding, drying, homogenization, weighing, digestion, filtration, dilution, etc., as well as data package documentation. The potential application of automation in sample preparation is extensive, in view of the need for all soil and water samples to undergo some of these steps before any subsequent analysis. As to data package documentation, it is required for any remedial and waste verification reporting.

Close collaboration with industry in the above niche areas is essential. In addition, the roles of a local champion to help penetrate the DOE market cannot be overly emphasized. The continued engagement of user champions to unveil or provide directions for niche development will lead to a better prospect of getting DOE sites to recognize that the future of chemical analyses lies in analysis automation.

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